

# A Review for the Time Integration of Semi-Linear Stiff Problems

Zainal Abdul Aziz<sup>1</sup>, Nazeeruddin Yaacob<sup>2</sup>, Mohammadreza Askaripour Lahiji<sup>3</sup>,  
Mahdi Ghanbari<sup>4</sup>

<sup>1,2,3</sup>Department of Mathematics, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Skudai,  
Johor, Malaysia

<sup>4</sup>Department of Mathematics, Islamic Azad University, Khorramabad Branch

## ABSTRACT

Several real-world requests that involve conditions where different physical phenomena perform on very different time scales arise simultaneously. The partial differential equations (PDEs) that manage such situations are classified as stiff PDEs. Stiffness is a difficult property of differential equations (DEs) that avoid conservative explicit numerical integrators from managing problem efficiency. There has also been a large compact of importance in the building of exponential integrators. However, different some of the new literature proposes, integrators based on this philosophy have been confirmed since at least 1960. The aim of this study is to review the time integration proposed for semi-linear stiff problems.

**KEYWORDS:** Exponential methods, numerical inverse Laplace transform, semi-linear parabolic equation.

## 1. INTRODUCTION

The theory of numerical methods for the time integration of semi-linear stiff problems is well-proposed by the application of exponential methods. Cox and Matthews (2002) studied a clear derivation of the explicit Exact Linear Part (ELP) method, from which they referred the methods as Exponential Time Differencing (ETD) and their implementation of the ETD methods. A modification of the ETD Runge-Kutta schemes of Cox and Matthews has been claimed by Kassman and Terfethen (2005). Maria Lopez-Fernandez (2004) discussed a new algorithm for the implementation of exponential methods, and the algorithm evaluates the operator by the exponential methods with a quadrature formula that is converges. A spectral order method for inverting sectorial Laplace transforms was studied by Maria Lopez-Fernandez et al. (2006). Moreover, the class of explicit multistep exponential and the explicit exponential Runge-Kutta methods were discussed by Hochbruck and Ostermann (2005). A representation for operators required in the implementation of these integrators in term of suitable Laplace transforms was proposed by Lopez-Fernandez et al. (2005). Other papers on this subject include [1, 4, 5, 7, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25].

The problems under consideration can be written as follows:

$$u'(t) = Au(t) + f(t, u(t)) \quad u(0) = u_0 \quad 0 \leq t \leq T, \quad (1)$$

where  $A$  is a linear operator that represents the highest order of differential terms and  $f$  is a lower under nonlinear operator. The variation of constants formula is considered for the solution to the initial value problem (1).

In Section 2, multistep exponential methods are discussed. In Section 3, exponential Runge-Kutta methods are proposed. In Section 4, evaluation of the mapping required is constructed by the multistep and the Runge-Kutta methods. In Section 5, numerical illustration is presented. Finally, the result is presented.

## 2. MULTISTEP EXPONENTIAL METHODS

The time integration of problems (1) is demonstrated by a class of explicit exponential methods [16]. with  $A : D(A) \subset X \rightarrow X$  the infinitesimal generator of a  $C_0$ -semi group  $e^{tA}$ ,  $t \geq 0$ , of linear bounded operators in a Banach space  $X$  [7]. The case of  $A$  in (1) is sectorial, i.e.,  $A$  is a densely defined and closed linear operator on  $X$  and there exists constants  $M > 0$ ,  $\gamma \in \mathbb{R}$ , and an angle  $0 < \delta < \frac{\pi}{2}$ , such that the resolvent fulfils

$$\|(zI - A)^{-1}\| \leq \frac{M}{|z - \gamma|} \quad \text{for } |\arg(z - \gamma)| < \pi - \delta. \quad (2)$$

Then, for  $0 \leq u < 1$ , the fractional powers  $(\omega - A)^\alpha$  are defined for  $\omega > \gamma$ , and  $X_\alpha = D((\omega - A)^\alpha)$  endowed with the graph norm  $\|\cdot\|_\alpha$  is a Banach space [7]. The nonlinearity  $f$  in (1) is supposed to be defined on

$[0, T] \times X_\alpha \rightarrow X$ , for some

$0 \leq \alpha < 1$ , and to be locally Lipschitz in a strip along the exact solution. Therefore, there exists  $L(R, T) > 0$  such that

\*Corresponding authors: Mohammadreza Askaripour Lahiji, Department of Mathematics, Faculty of Science, University Teknologi Malaysia, 81310 UTM Skudai, Johor, Malaysia. Email: maskarepor@yahoo.com

$$\|f(t, \gamma) - f(t, \xi)\| \leq L \|\gamma - \xi\|_a \quad \gamma, \xi \in X_a, \quad 0 \leq t \leq T, \quad (3)$$

for  $\max(\|\gamma - u(t)\|_a, \|\xi - u(t)\|_a) \leq R$ .

The variation of constants formula in interval  $[t_n, t_{n+k}]$  is presented for  $k$ -step method ( $k \geq 1$ ).

Setting a step size  $h = T/N$ ,  $N \geq k$ , and the corresponding time levels  $t_n = nh$ ,

$0 \leq n \leq N$ , the solution (1) at  $t_{n+k}$  is given by

$$u(t_{n+k}) = u(t_n) e^{k\lambda A} + h \int_0^k e^{(k-\sigma)\lambda A} f(t_n + \sigma h, u(t_n + \sigma h)) d\sigma \quad (4)$$

Given approximations  $u_{n+j} \approx u(t_{n+j})$ ,  $0 \leq j \leq k-1$ , after replacing  $f$  in (4) by the Lagrange interpolation polynomial of degree  $k-1$ ,  $P_{n,k-1}$  through the points  $\{(t_{n+j}, f(t_{n+j}, u_{n+j}))\}_{j=0}^{k-1}$  and integrating, the approximation  $u_{n+k} \approx u(t_{n+k})$  is obtained.

$$P_{n,k-1}(t_n + \sigma h) = \sum_{j=0}^{k-1} \omega_j^{(k)}(\sigma) \Delta^j f_n, \quad (5)$$

with  $f_m = f(t_m, u_m)$ ,  $0 \leq m \leq N-1$ , and  $\Delta$  the standard forward difference from

$$u_{n+k} = \phi_0(k, hA) u_n + h \sum_{j=0}^{k-1} \phi_{j+1}(k, hA) \Delta^j f_n, \quad (6)$$

where

for  $\ell \in \mathbb{C}$ ,  $k \geq 1$ ,  $0 \leq j < k$ , and  $\phi_j(k, \lambda)$  are given by

$$\begin{aligned} \phi_j(k, \lambda) &= \int_0^k e^{(k-\sigma)\lambda} \omega_{j-1}^{(k)}(\sigma) d\sigma, \quad 1 \leq j \leq k \\ \phi_0(k, \lambda) &= e^{k\lambda}, \end{aligned} \quad (7)$$

The methods considered in (6) are explicit and they require the evaluation  $\phi_j(k, hA)$ .

### 3. EXPONENTIAL RUNGE-KUTTA METHODS

In the time integration of semi-linear parabolic problems, explicit exponential Runge-Kutta methods have been demonstrated [6, 10].

For  $h = T/N$ ,  $N \geq 1$ , and  $1 \leq i \leq s$ , the approximation  $u_n$  to  $u(t_n)$ , with  $t_n = nh$ , are presented by

$$U_{n1} = u_n e^{c_1 h A} + h \sum_{j=1}^{i-1} a_{ij}(hA) f(t_n + c_j h, U_{nj}), \quad (8)$$

$$u_{n+1} = u_n e^{hA} + h \sum_{i=1}^s b_i(hA) f(t_n + c_i h, U_{ni}),$$

with  $c_1 = 0$  ( $U_{n1} = u_n$ ).

The coefficients  $b_i(\lambda)$  and  $a_{ij}(\lambda)$  are linear combinations of  $\varphi_k(\lambda)$  and  $\varphi_k(c_i \lambda)$  with

$$\varphi_k(\lambda) = \int_0^1 e^{(1-\sigma)\lambda} \frac{\sigma^{k-1}}{(k-1)!} d\sigma, \quad \lambda \in \mathbb{C}, k \geq 1, t > 0. \quad (9)$$

Take  $\varphi_0(\lambda) = e^\lambda$ . The implementing of (8) requires the evaluation of  $\varphi_k(hA)$  and  $\varphi_k(c_i hA)$ , for  $1 \leq i \leq s$  and several values of  $k \geq 0$ . Besides, the nonlinearity  $f$  in (1) has satisfied a local Lipchitz condition [16].

#### 4. Evaluation of the vector-valued mapping

Some Laplace transformation formulas are used for getting a suitable representation of the operators  $\phi_j(k, hA)$ ,  $\varphi_j(hA)$ , and  $\varphi_j(c_i hA)$  applied in (6) and (8). For a locally integral mapping  $f: (0, \infty) \rightarrow X$ , bounded by

$$\|f(t)\| \leq C t^{\nu-1} e^{\gamma t}, \quad \text{for some } \gamma, \nu > 0.$$

For some  $\gamma, \nu > 0$ , the Laplace transform is noted by

$$F(z) = L[f](z) = \int_0^\infty e^{-tz} f(t) dt, \quad \operatorname{Re}(z) > \gamma.$$

The inverse transform is achieved by means of a suitable rule to discretize the inversion formula

$$f(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} F(z) dz,$$

where  $\Gamma$  is a contour in the complex plan, running from  $-i\infty$  to  $i\infty$  and laying in the analytical region of  $F$ , and it is noted that  $f(\sigma) = L^{-1}[F](\sigma)$  [8, 9, 11, 12, 13].

#### 4.1 Evaluation of the mapping required by the multistep methods

For  $\phi_j$  in (7) with  $1 \leq j \leq k$ , it is considered [8, 9, 15]

$$\phi_j(k, \lambda) = \int_0^k e^{(k-\sigma)\lambda} \binom{\sigma}{j-1} d\sigma = L^{-1} \left[ L[f_0(\cdot, \lambda)] \times L[f_j] \right](k),$$

where, for  $\sigma \geq 0$ ,

$$f_0(\sigma, \lambda) = e^{\sigma\lambda} \text{ and } f_j(\sigma) = \binom{\sigma}{j-1}. \quad (10)$$

For every  $j \geq 1$  and  $z \in \mathbb{C}$ , the following formula is defined as

$$\Psi_j(z, \lambda) = L[f_0(\cdot, \lambda)](z) \times L[f_j](z) = \frac{1}{z-1} \times L[f_j](z). \quad (11)$$

Thus, for every  $\lambda \in \mathbb{C}$  and  $j \geq 1$ ,

$$\phi_j(k, \lambda) = L^{-1}[\Psi_j(z, \lambda)](k). \quad (12)$$

For  $j = 0$

$$\phi_0(k, \lambda) = e^{k\lambda} = L^{-1}\left(\frac{1}{z-\lambda}\right)(k),$$

and thus the following formula is defined

$$\Psi_0(z, \lambda) = \frac{1}{z-\lambda}. \quad (13)$$

For  $\lambda$  scalar, the mappings  $\Psi_j(z, \lambda)$ , with  $1 \leq j \leq 4$  are presented by

$$\begin{aligned} \Psi_1(z, \lambda) &= \frac{1}{z(z-\lambda)}, & \Psi_2(z, \lambda) &= \frac{1}{z^2(z-\lambda)}, \\ \Psi_3(z, \lambda) &= \frac{z-z^2}{z^2(z-\lambda)}, & \Psi_4(z, \lambda) &= \frac{z-2z^2+z^3}{z^2(z-\lambda)}. \end{aligned} \quad (14)$$

In order to evaluate  $\phi_j(k, hA)$ ,  $1 \leq j \leq 4$ , the formulas (14) with  $hA$  instead of  $\lambda$  are proposed. For approximating the original mapping at  $\sigma = k$ , the inversion of the Laplace transform has been performed [8, 9]. In this way, the following formulas are invert of Laplace transforms that we need:

$$\begin{aligned} \Psi_0(z, hA) &= (zI - hA)^{-1}, \\ \Psi_1(z, hA) &= \frac{1}{z} (zI - hA)^{-1}, \\ \Psi_2(z, hA) &= \frac{1}{z^2} (zI - hA)^{-1}, \\ \Psi_3(z, hA) &= \frac{z-2}{z^2} (zI - hA)^{-1}, \\ \Psi_4(z, hA) &= \frac{z-2z+z^2}{z^2} (zI - hA)^{-1}. \end{aligned} \quad (15)$$

Note that because of (2), the mapping  $\Psi(z, hA)$  turns out to be sectorial in the variable  $z$ , i.e., there exists constants  $\gamma \in \mathbb{R}$  and  $M > 0$ , possibly different form of the constants in (2), such that

$\Psi(z, hA)$  is analytic for  $z$  in the sector  $|\arg(z - \gamma)| < \pi - \delta$  and there

$$\|\Psi(z, hA)\| \leq \frac{M}{|z-\gamma|^v}, \quad \text{for some } v \geq 1. \quad (16)$$

The formulas in (15) can also be considered by combining the Cauchy integral formula [7, 8, 14] with the inversion formula for Laplace transform. For suitable contours  $\Gamma_1$  and  $\Gamma_2$  in the complex plan, both of them lay the resolvent set of  $A$ , which holds

$$\begin{aligned} \phi_j(k, hA) &= \frac{1}{2\pi i} \int_{\Gamma_1} \phi_j(k, \lambda) (\lambda I - hA)^{-1} d\lambda \\ &= \frac{1}{2\pi i} \int_{\Gamma_1} \left( \frac{1}{2\pi i} \int_{\Gamma_2} e^{k\xi} \Psi_j(\xi, \lambda) d\xi \right) (\lambda I - hA)^{-1} d\lambda \\ &= \frac{1}{2\pi i} \int_{\Gamma_2} e^{k\xi} \left( \frac{1}{2\pi i} \int_{\Gamma_1} \Psi_j(\xi, \lambda) (\lambda I - hA)^{-1} d\lambda \right) d\xi \\ &= \frac{1}{2\pi i} \int_{\Gamma_2} e^{k\xi} \Psi_j(\xi, hA) d\xi = L^{-1}[\Psi_j(\cdot, hA)](k). \end{aligned} \quad (17)$$

#### 4.2 Evaluation of the mapping by the Runge-Kutta methods

For  $\varphi_j$  in (9),  $j \geq 1$  and  $t \geq 0$ , the following formula is considered [8, 9, 15]

$$\varphi_j(\lambda) = \int_0^1 e^{(1-\sigma)\lambda} \frac{\sigma^{j-1}}{(j-1)!} d\sigma = L^{-1} \left[ L[g_0(\cdot, \lambda)] \times L[g_j] \right](1),$$

where for  $\sigma \geq 0$ ,  $\lambda \in \mathbb{C}$ ,

$$g_0(\sigma, \lambda) = e^{\sigma\lambda} \text{ and } g_j(\sigma) = \frac{\sigma^{j-1}}{(j-1)!}. \quad (18)$$

For every  $j \geq 1$  and  $\lambda \in \mathbb{C}$ , the following formula is defined

$$\Phi_j(x, \lambda) = L[g_0(x, \lambda)](x) \times L[g_j](x) = \frac{1}{x^j(x-\lambda)}, \quad (19)$$

and  $\Phi_0(x, \lambda) = (x - \lambda)^{-1}$ . Then, for every  $\lambda \in \mathbb{C}$  and  $j \geq 0$ ,

$$\varphi_j(\lambda) = L^{-1}[\Phi_j(x, \lambda)](1). \quad (20)$$

The same as argument in (17) justifies the operators  $\varphi_j(hA)$  and  $\varphi_j(c_l hA)$ ,  $j \geq 0$ ,  $2 \leq l \leq s$ , which can be calculated by applying the inversion of the Laplace transforms

$$\Phi_j(x, \beta hA) = \frac{1}{x^j} (x - \beta hA)^{-1}, \quad j \geq 0, \quad \beta = 1, c_l, \quad (21)$$

to approximate the original mapping at  $\sigma = 1$  [8].

## 5. Numerical illustration

In this part, the same examples are proposed [6, 16].

### 5.1 Example for the multistep exponential methods

The following problem is demonstrated [16]

$$u_t(x, t) = u_{xx}(x, t) + \left( \int_0^1 u(s, t) ds \right) u_x(x, t) + g(x, t), \quad (22)$$

for  $x \in [0, 1]$  and  $t \in [0, 1]$ , subject to homogeneous Dirichlet boundary conditions and with  $g(x, t)$  such that the exact solution to (22) is  $u(x, t) = x(1-x)e^t$ . Moreover, in the example, the mapping

$$\varphi(\lambda) = \frac{e^{\lambda-1}}{\lambda}, \quad (23)$$

is considered [8].

$\lambda < 0$	$K = 15$	$K = 25$	$-\lambda$	$K = 15$	$K = 25$
-1	1.5050e-12	1.3323e-15	1	1.5050e-12	3.3307e-15
-1e-1	1.5227e-12	3.2196e-15	1e-1	1.5227e-12	3.5527e-15
-1e-2	1.4243e-12	4.4409e-15	1e-2	1.4243e-12	4.6629e-15
-1e-3	1.3750e-12	1.3323e-15	1e-3	1.3750e-12	1.3323e-15
-1e-4	1.3738e-12	1.7764e-15	1e-4	1.3738e-12	1.7764e-15
-1e-5	1.3747e-12	3.6637e-15	1e-5	1.3747e-12	3.7748e-15
-1e-6	1.3748e-12	3.6637e-15	1e-6	1.3748e-12	3.7748e-15
-1e-7	1.3695e-12	1.9984e-15	1e-7	1.3695e-12	1.9984e-15
-1e-8	1.3717e-12	1.1102e-16	1e-8	1.3717e-12	2.2204e-16
-1e-9	1.3715e-12	1.1102e-16	1e-9	1.3715e-12	0
-1e-10	1.3711e-12	0	1e-10	1.3711e-12	0
-1e-11	1.3711e-12	0	1e-11	1.3711e-12	0
-1e-12	1.3715e-12	1.1102e-16	1e-12	1.3715e-12	0
-1e-13	1.3712e-12	0	1e-13	1.3712e-12	2.2204e-16

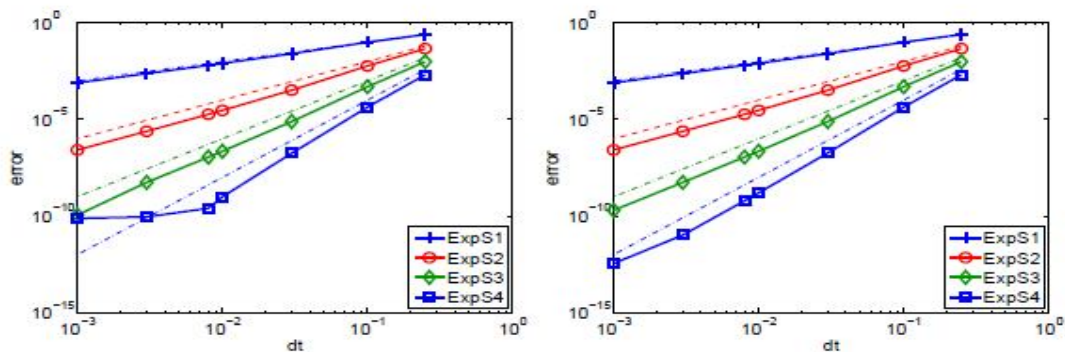
**Table 1:**  $\varphi(\lambda)$  in (23) for  $\lambda \in [-1, 1]$  is computed, and the absolute error obtained is displayed by MATLAB with  $K = 15$  and  $K = 25$ .

In the table, the spatial discretization of (22) is implemented by applying standard finite differences with  $J = 512$  spatial nodes, centered for the approximation of  $u_x$ .

The nonlocal term has been presented by the composite Simpson's formula [16]. Moreover, the formula (6) is utilised with  $k = 1, 2, 3, 4$ , for integrating in time the semi discrete problem so that  $A$  is  $(J-1) \times (J-1)$  matrix

$$A = J^2 \text{tridiag}([1, -2, 1]).$$





**Figure 1:** Error of exponential multistep methods (6) utilised to (22), for  $k = 1, 2, 3$ , and 4. Left: With  $K = 25$  quadrature nodes on the hyperbolas, Right: With  $K = 35$ . In Figure 1, the error versus the step size at  $t = 1$  is shown and measured in a discrete version of the norm  $\|\cdot\|_{1/2}$ , for  $K = 25$  and  $K = 35$ . In Figure 1 also, lines of slope 1, 2, 3, and 4 are observed to visualise the order of convergence [16]. In fact, it is higher than the one predicted in [16].

## 5.2 Example of the exponential Runge-Kutta methods

In this section, two examples are proposed [6]. The first following problem is considered [6]

$$u_t(x, t) = u_{xx}(x, t) + \frac{1}{1+u(x, t)^2} + g(x, t), \quad (24)$$

for  $x \in [0, 1]$  and  $t \in [0, 1]$ , subject to homogeneous Dirichlet boundary conditions and with  $g(x, t)$  such that the exact solution to (24) is  $u(x, t) = x(1-x)e^t$ . Moreover, the Butcher tableaux are applied with the abbreviations

$$\varphi_i = \varphi_i(hA), \quad \text{and } \varphi_{i,j} = \varphi_{i,j}(hA) = \varphi_i(c_j hA), \quad 2 \leq j \leq s.$$

This problem is discretised in space by standard finite differences with  $J = 200$  grid points. For the time integration of semidiscrete problem, the equations (8) are considered with method

$$\begin{array}{c|c} 0 & \\ \hline \frac{1}{2} & \frac{1}{2}\varphi_{1,2} \\ \hline & 0 \quad \varphi_1 \end{array} \quad (25)$$

the third-order method

$$\begin{array}{c|ccc} 0 & & & \\ \hline \frac{1}{3} & \frac{1}{3}\varphi_{1,2} & & \\ \frac{2}{3} & \frac{2}{3}\varphi_{1,3} - \frac{4}{3}\varphi_{2,3} & \frac{4}{3}\varphi_{2,3} & \\ \hline & \varphi_1 - \frac{3}{2}\varphi_2 & 0 & \frac{3}{2}\varphi_2 \end{array} \quad (26)$$

and the fourth-order method

$$\begin{array}{c|cccc} 0 & & & & \\ \hline \frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & & \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,3} - \varphi_{2,3} & \varphi_{2,3} & & \\ 1 & \varphi_{1,4} - 2\varphi_{2,4} & \varphi_{2,4} & \varphi_{2,4} & \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,5} - 2a_{5,2} - a_{5,4} & a_{5,2} & a_{5,2} & a_{5,4} \\ \hline & \varphi_1 - 3\varphi_2 + 4\varphi_3 & 0 & 0 & -\varphi_2 + 4\varphi_3 \quad 4\varphi_2 - 8\varphi_3 \end{array} \quad (27)$$

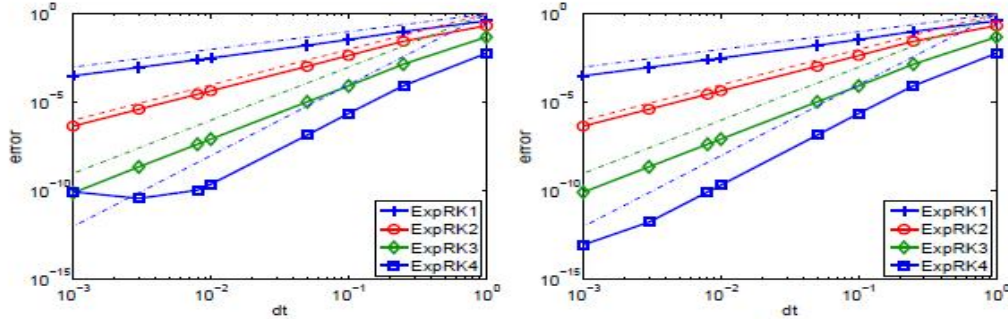
with

$$a_{5,2} = \frac{1}{2}\varphi_{2,5} - \varphi_{3,4} + \frac{1}{4}\varphi_{2,4} - \frac{1}{2}\varphi_{3,5}$$

and

$$a_{5,4} = \frac{1}{4}\varphi_{2,5} - a_{5,2}.$$

In the implementation of the second order method, to invert four different Laplace transforms, the form of (21) is needed for approximating  $\varphi_0(\frac{h}{2}A)$ ,  $\varphi_0(hA)$ ,  $\varphi_1(\frac{h}{2}A)$ , and  $\varphi_1(hA)$ . In addition, the inversion of eight Laplace transforms is required in the implementation of the third-order and fourth-order methods.



**Figure 2:** Error of Runge-Kutta methods (8) with  $s = 1$ , (25), (26), and (27) utilized to (24).

Left: With  $K = 25$  quadrature nodes, Right:  $K = 35$ .

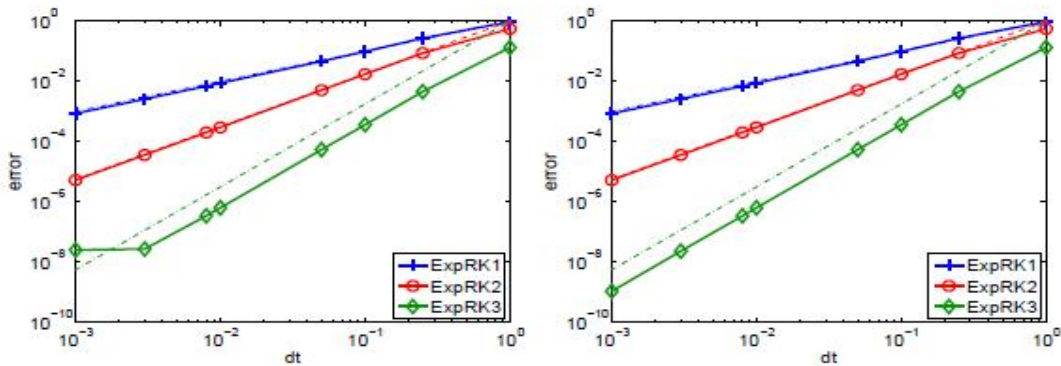
In Figure 2, the error at  $t = 1$  versus the step size is displayed and measured in the maximum norm. In order to test the algorithm, lines with the corresponding slopes in Figure 2 are added. For this kind of methods, full precision for  $K = 35$  are seen [6].

The second following problem is presented [6]

$$u_t(x, t) = u_{xx}(x, t) + \int_0^1 u(s, t) ds + g(x, t), \quad (28)$$

for  $x \in [0, 1]$  and  $t \in [0, 1]$ , subject to homogeneous Dirichlet boundary conditions and with  $g(x, t)$  such that the exact solution to (28) is  $u(x, t) = x(1 - x)e^t$ .

This problem in space is discretized as in the previous example (22), and the composite Simpson's rule is applied for the approximation of the nonlocal term. For the time integration, the formulas (8) are used with  $s = 1$ , (25), and (26).



**Figure 3:** Error of Runge-Kutta methods (8) with  $s = 1$ , (25), and (26) applied to (28).

Left: With  $K = 20$  quadrature nodes, Right: With  $K = 25$ .

In Figure 3, the error at  $t = 1$  is shown and measured in a discrete version of the norm  $\|\cdot\|_{1/2}$  [6]. The order of convergence for this problem is expected, where the first order is 1, 1.75 for (25), and 2.75 for (26). Lines with the corresponding slopes in Figure 3 are added in order to check the algorithm for exponential methods. Full precision with only  $K = 25$  quadrature nodes is achieved [6].

## 6. Conclusions

In this work, the way to approximate the exponential operators required for the implementation of different kinds of exponential methods has been derived, which have been demonstrated for the time integration of semi-linear problems. Moreover, the numerical inversion of the Laplace transform and its applications have been shown. Two examples of the multistep exponential and the exponential Runge-Kutta methods have also been considered.

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